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Stochastic Partial Differential Equations

Predictive Modeling – Coping with Uncertainty

D.M. Tartakovsky*, Los Alamos National Laboratory
A. Guadagnini, Politecnico di Milano

Summary

Our ability to make accurate predictions of the behavior of most physical and social systems is often hampered by the lack of sufficient data. Recent advances in the theory and application of stochastic partial differential equations provide a powerful tool for coping with the uncertainty that arise from our limited knowledge of such systems.

Although it has long been recognized that simulations of most physical systems are fundamentally stochastic, this fact remains overlooked in most practical applications. Even essentially deterministic systems must be treated stochastically when their parameters are under-specified by data. Parameter uncertainty limits our ability to accurately simulate and predict the manufacturing of composite materials, scaling in condensed and soft matter, earthquakes and seismic monitoring, reservoir exploitation, environmental remediation, and other complex systems important to the core mission of the Department of Energy.

To improve our ability to predict the dynamics of systems with limited data, we have assembled an interdisciplinary team of researches from applied mathematics, statistics and scientific computing. Our research has led to new approaches that improve the accuracy of the predictions and give tighter bounds on uncertainty arising from stochastic simulations of physical system states and parameters.

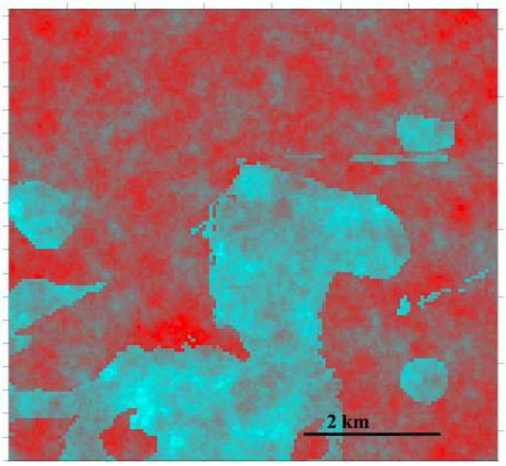
We have developed a method of random domain decomposition (RDD) that provides a novel doubly stochastic model to quantify the impact of the type of spatially heterogeneous random processes that typically appear in realistic simulations of physical systems. The problem domain is decomposed according to stochastic geometries into disjoint random fields. The stochastic decomposition is determined by variations in the parameter space based on additional (uncertain) geometric information that can be derived from new characterization techniques and also from expert knowledge.

Previous work has tended to concentrate on spatially homogeneous parameterizations, or at most on heterogeneous parameter fields whose geometry is assumed known with certainty. This is almost never the case in natural systems. RDD allows scientists to predict the behavior of multiscale systems with heterogeneous parameterizations that depend on realistic geometric uncertainty.

RDD has also led to new approaches for reconstructing images from sparse and noisy

* (505) 667-0968, dmt@lanl.gov

data. In addition to providing a best estimate of an image, RDD yields its probabilistic description.



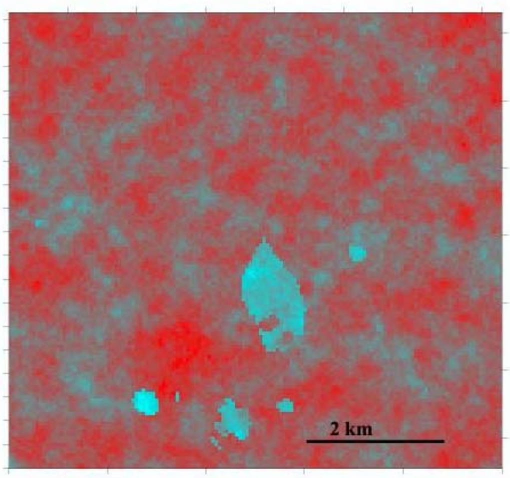


Figure 1. Porous media composed of two heterogeneous materials, one of high (turquoise) and the other of low (red) conductivity. The material distributions are reconstructed from a sparse geophysical data set. The top figure shows the boundary configuration corresponding to 74% probability of low conductivity occurrence. The bottom figure provides a more conservative estimate of the boundary configuration (87% probability of low probability occurrence).

One application, where RDD has already made a significant impact, is contaminant transport in subsurface environments. Such environments are notoriously heterogeneous and their characterizations are highly costly and often inaccurate. Since contaminants tend to move through highly conductive regions, it is paramount to identify them from available data. Since such data are scarce, it is important to quantify uncertainties in our predictions in terms of the uncertainty of the data, and to evaluate the corresponding risks.

Figure 1 shows an example of a boundary between two heterogeneous materials computed from available data with various degrees of certainty. The turquoise regions serve as contaminant conduits in the otherwise impermeable rock that is shown in red. Note that as our predictions become more conservative (i.e. have higher probability of low conductivity occurrence), the size of the highly conductive regions diminishes.

Combined with the probabilistic image reconstruction, RDD has allowed us to make predictions of physical processes, such as fluid flow, occurring in this composite medium with accuracy not attainable by other approaches.

Our future research efforts in predictability of physical systems in complex heterogeneous environments will involve developing (i) state-of-the-art statistical techniques for parameter estimation and probabilistic image reconstruction, (ii) new methods of analysis of stochastic partial differential equations, and (iii) efficient methods for their numerical implementation.

For further information on this subject contact:
Dr. Charles H. Romine, Program Manager
Applied Mathematical Sciences Division
Office of Advanced Scientific Computing Research
Phone: 301-903-5152
romine@er.doe.gov